

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF092421\  
 Data File : BF125628.D  
 Acq On : 24 Sep 2021 19:13  
 Operator : JU/CG  
 Sample : M3911-03  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SW-RR-03-(SA)

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF092421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125628.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 2.199       | 12            | 19          | 24           | rVB      | 3752240        | 4909505       | 76.74%          | 13.011%       |
| 2         | 5.498       | 576           | 580         | 584          | rBV      | 2534953        | 2478902       | 38.75%          | 6.570%        |
| 3         | 6.498       | 746           | 750         | 753          | rBV      | 1866948        | 1570077       | 24.54%          | 4.161%        |
| 4         | 6.887       | 812           | 816         | 819          | rBV      | 1349199        | 1116031       | 17.44%          | 2.958%        |
| 5         | 7.445       | 905           | 911         | 914          | rBV      | 3309805        | 3355926       | 52.46%          | 8.894%        |
| 6         | 8.063       | 1012          | 1016        | 1022         | rBV      | 174013         | 154572        | 2.42%           | 0.410%        |
| 7         | 8.169       | 1029          | 1034        | 1036         | rBV      | 1748744        | 1576502       | 24.64%          | 4.178%        |
| 8         | 9.245       | 1211          | 1217        | 1220         | rBV      | 6889429        | 6397703       | 100.00%         | 16.955%       |
| 9         | 9.922       | 1327          | 1332        | 1335         | rVB      | 2260105        | 1818372       | 28.42%          | 4.819%        |
| 10        | 10.710      | 1461          | 1466        | 1469         | rBV      | 4078049        | 3731516       | 58.33%          | 9.889%        |
| 11        | 10.798      | 1476          | 1481        | 1484         | rBV      | 193474         | 176743        | 2.76%           | 0.468%        |
| 12        | 11.404      | 1580          | 1584        | 1588         | rBV      | 2154316        | 1790057       | 27.98%          | 4.744%        |
| 13        | 11.927      | 1667          | 1673        | 1685         | rBV3     | 212367         | 287623        | 4.50%           | 0.762%        |
| 14        | 12.710      | 1801          | 1806        | 1818         | rBV      | 110301         | 166795        | 2.61%           | 0.442%        |
| 15        | 12.992      | 1849          | 1854        | 1857         | rBV      | 5807485        | 5639746       | 88.15%          | 14.947%       |
| 16        | 13.221      | 1885          | 1893        | 1896         | rBV9     | 32163          | 74977         | 1.17%           | 0.199%        |
| 17        | 13.263      | 1896          | 1900        | 1916         | rVB9     | 42588          | 144420        | 2.26%           | 0.383%        |
| 18        | 13.886      | 2000          | 2006        | 2008         | rBV2     | 84467          | 128090        | 2.00%           | 0.339%        |
| 19        | 14.039      | 2028          | 2032        | 2036         | rBV      | 1292168        | 1088543       | 17.01%          | 2.885%        |
| 20        | 15.515      | 2277          | 2283        | 2288         | rBV      | 906427         | 1126497       | 17.61%          | 2.985%        |

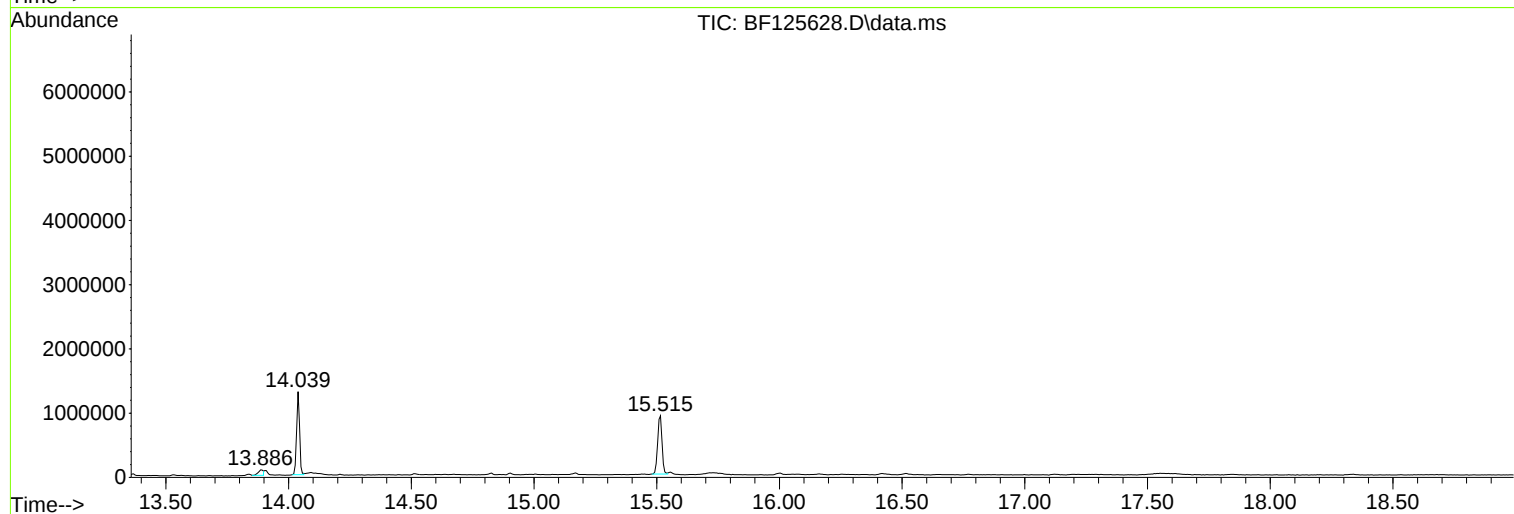
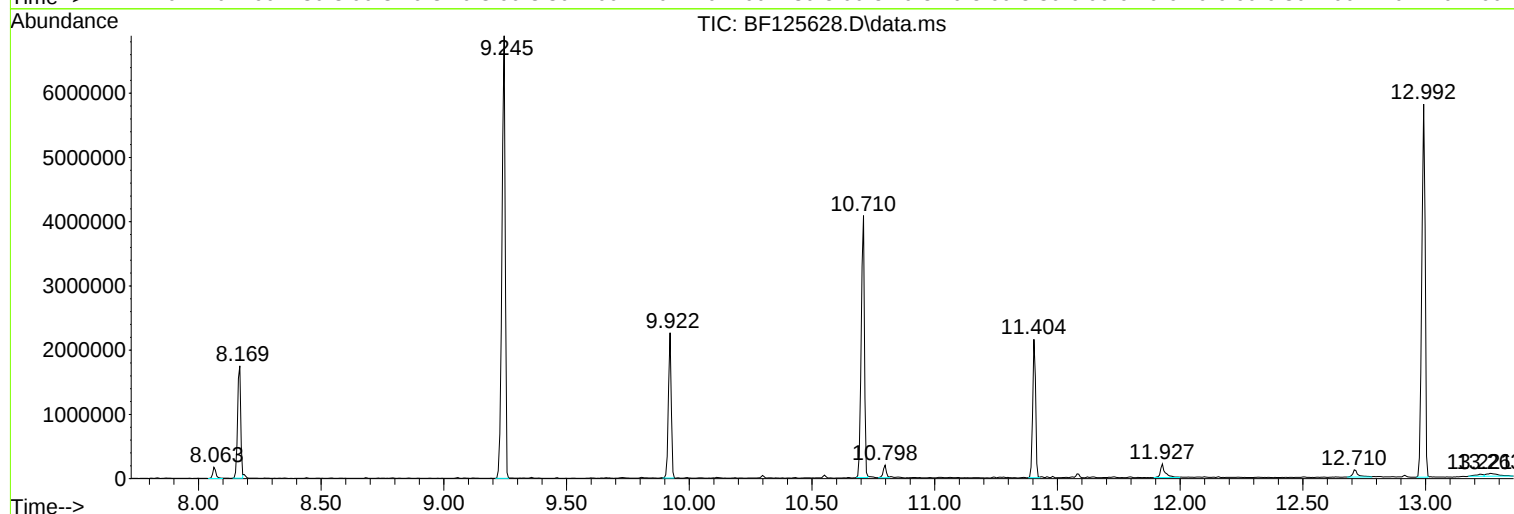
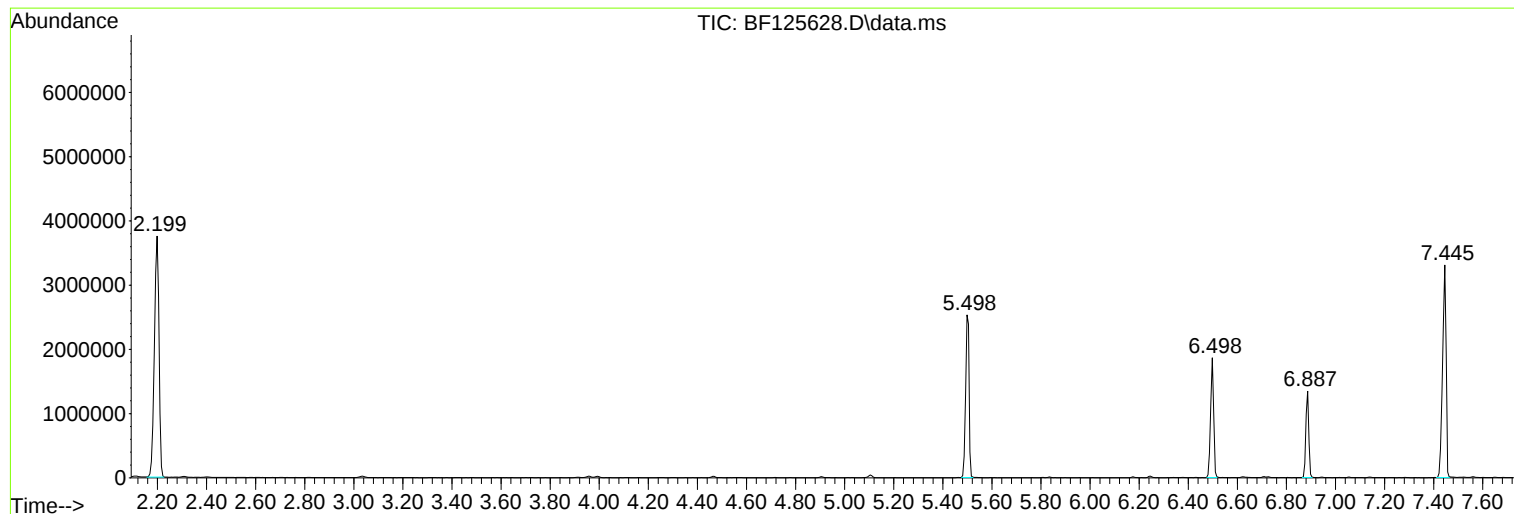
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Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF092421.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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ClientSampleId :  
SW-RR-03-(SA)

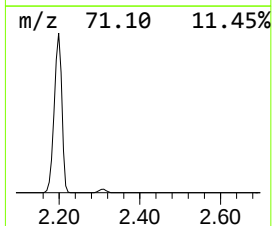
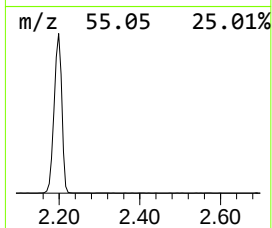
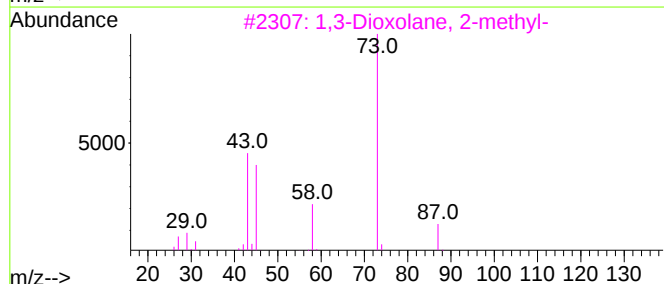
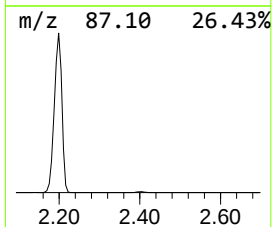
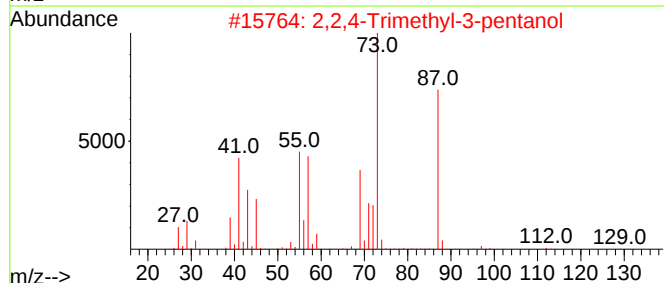
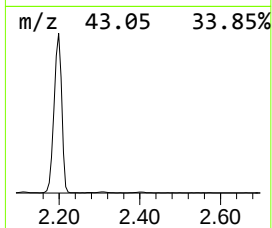
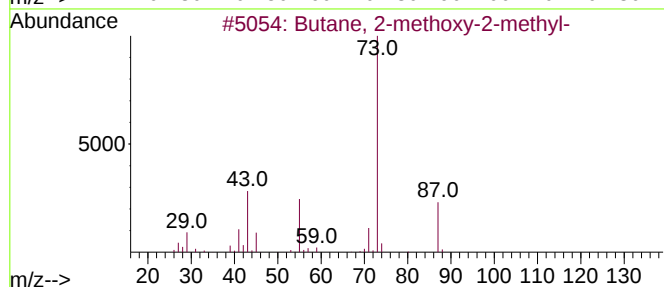
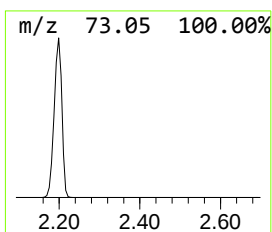
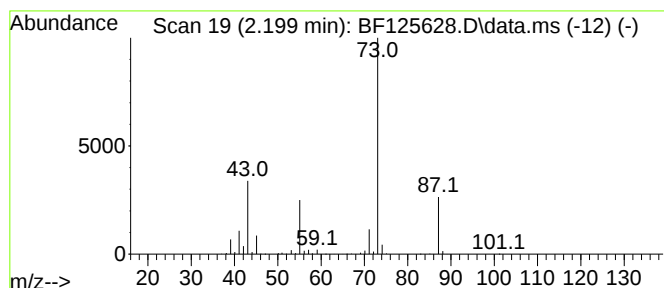
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF092421.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 2.199 | 87.98 ng | 4909510 | 1,4-Dichlorobenzene-d4 | 6.887 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 78   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 25   |
| 4    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 5    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 17   |



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Misc :  
ALS Vial : 5 Sample Multiplier: 1

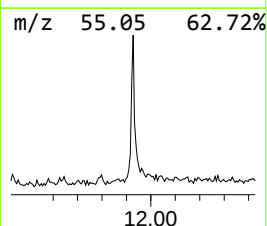
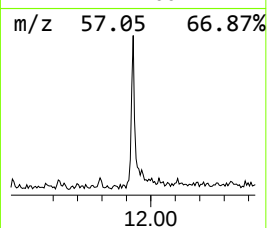
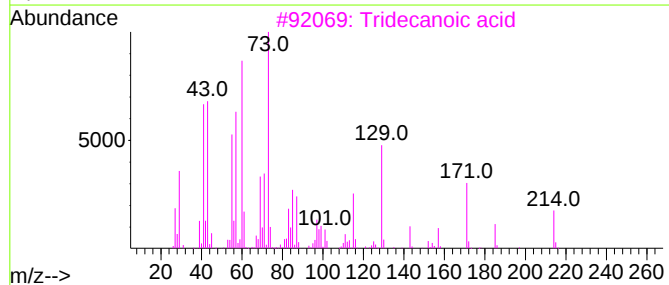
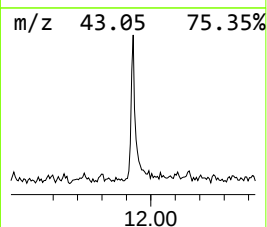
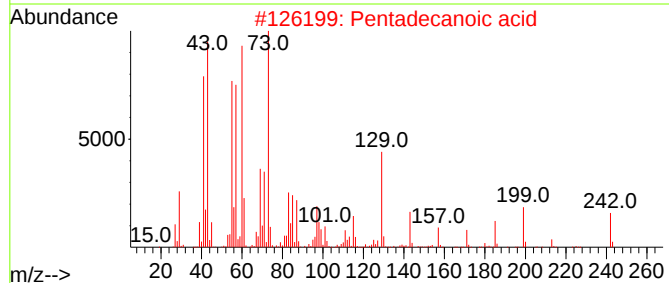
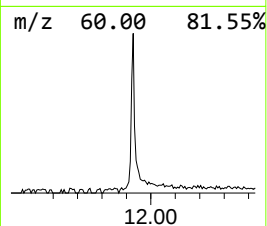
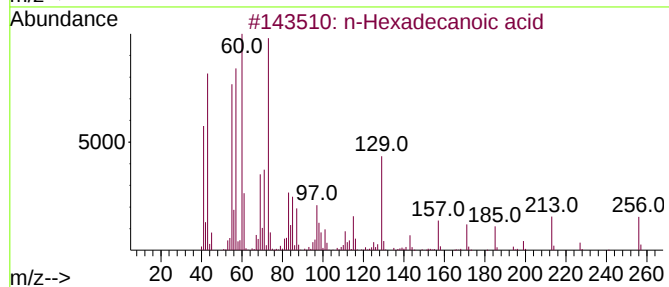
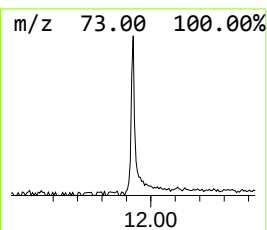
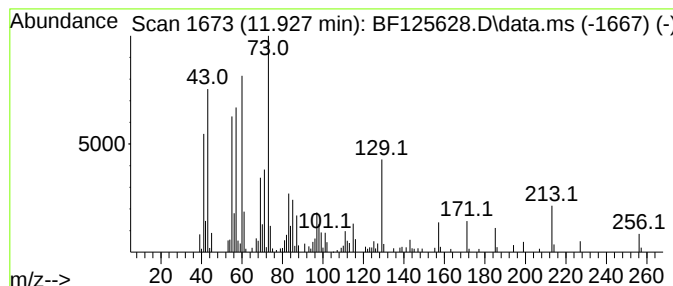
Instrument :  
BNA\_F  
ClientSampleId :  
SW-RR-03-(SA)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF092421.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

| R.T.      | EstConc             | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------|--------|------------------|-------------|------|
| 11.927    | 3.21 ng             | 287623 | Phenanthrene-d10 | 11.404      |      |
| Hit# of 5 | Tentative ID        | MW     | MolForm          | CAS#        | Qual |
| 1         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 99   |
| 2         | Pentadecanoic acid  | 242    | C15H30O2         | 001002-84-2 | 87   |
| 3         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 80   |
| 4         | Tetradecanoic acid  | 228    | C14H28O2         | 000544-63-8 | 74   |
| 5         | n-Decanoic acid     | 172    | C10H20O2         | 000334-48-5 | 70   |



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Sample : M3911-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SW-RR-03-(SA)

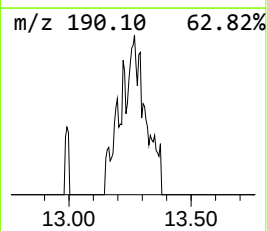
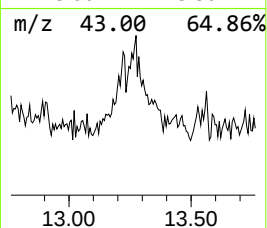
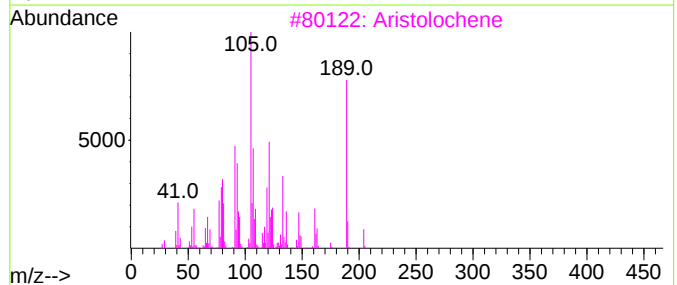
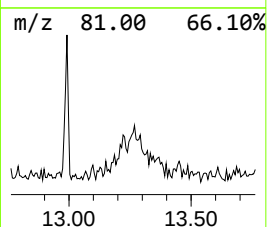
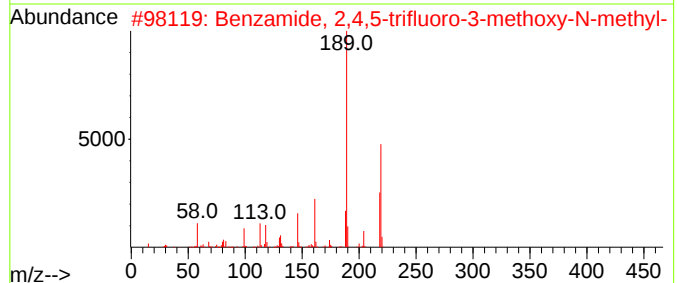
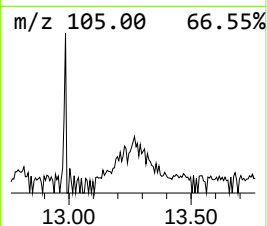
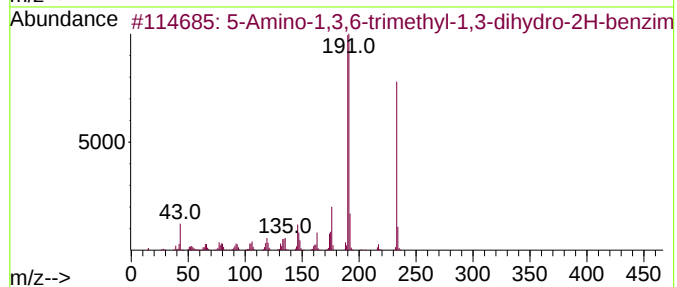
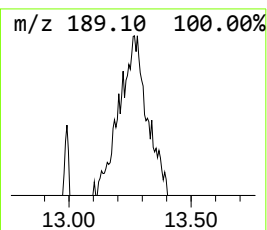
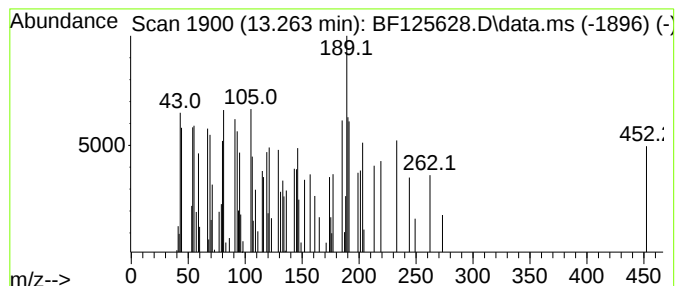
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown13.263 Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.263 | 2.65 ng | 144420 | Chrysene-d12     | 14.039 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 5-Amino-1,3,6-trimethyl-1,3-dihy... | 233 | C12H15N3O2 | 1031646-04-4 | 15   |
| 2    |    |   | Benzamide, 2,4,5-trifluoro-3-met... | 219 | C9H8F3NO2  | 1000407-63-4 | 14   |
| 3    |    |   | Aristolochene                       | 204 | C15H24     | 026620-71-3  | 11   |
| 4    |    |   | (3S,3aR,6R,8aS)-7,7-Dimethyl-8-m... | 218 | C15H22O    | 082509-29-3  | 10   |
| 5    |    |   | 2-Butenimidic acid, 3-methyl-N-p... | 189 | C12H15NO   | 056830-02-5  | 10   |



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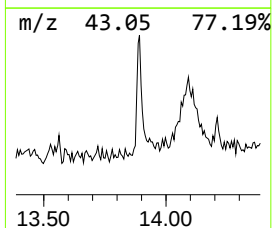
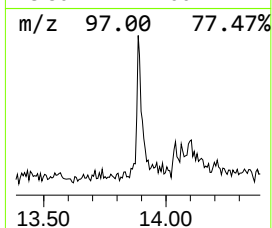
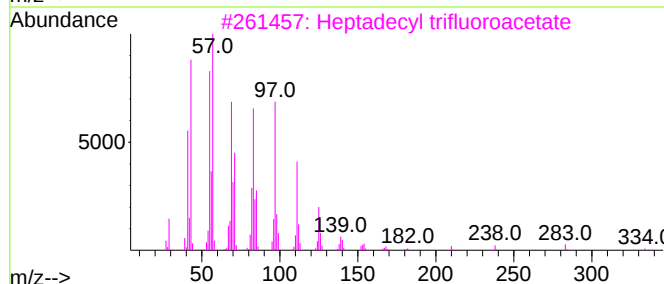
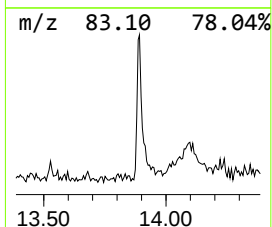
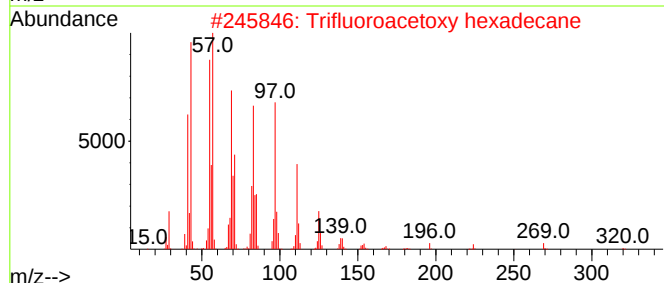
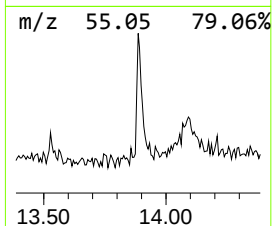
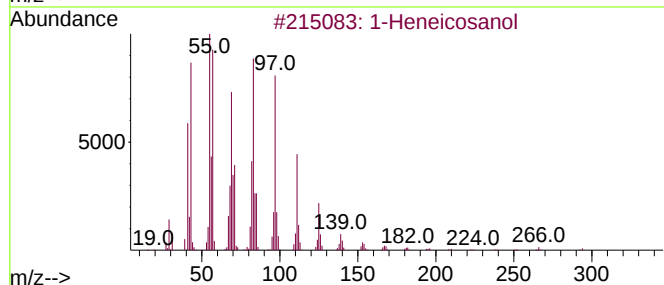
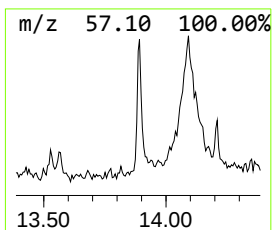
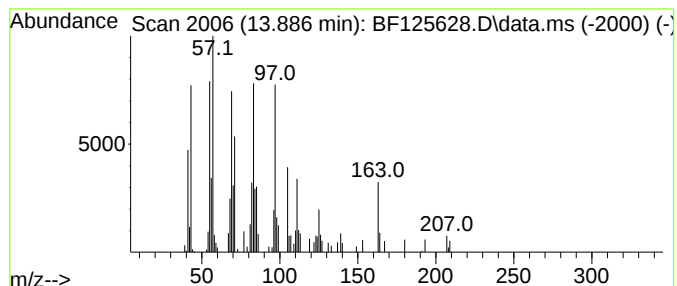
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TIC Library : C:\Database\NIST20.L  
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\*\*\*\*\*  
Peak Number 4 1-Heneicosanol Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.886 | 2.35 ng | 128090 | Chrysene-d12     | 14.039 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-----------------------------|-----|------------|--------------|------|
| 1    |    |   | 1-Heneicosanol              | 312 | C21H44O    | 015594-90-8  | 93   |
| 2    |    |   | Trifluoroacetoxy hexadecane | 338 | C18H33F3O2 | 006222-03-3  | 93   |
| 3    |    |   | Heptadecyl trifluoroacetate | 352 | C19H35F3O2 | 1010351-87-0 | 93   |
| 4    |    |   | 1-Hexacosene                | 364 | C26H52     | 018835-33-1  | 90   |
| 5    |    |   | 1-Hexacosanol               | 382 | C26H54O    | 000506-52-5  | 90   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Butane, 2-metho... | 2.199  | 88.0    | ng    | 4909510  | 1                     | 6.887  | 1116030 | 20.0 |
| n-Hexadecanoic ... | 11.927 | 3.2     | ng    | 287623   | 4                     | 11.404 | 1790060 | 20.0 |
| unknown13.263      | 13.263 | 2.6     | ng    | 144420   | 5                     | 14.039 | 1088540 | 20.0 |
| 1-Heneicosanol     | 13.886 | 2.4     | ng    | 128090   | 5                     | 14.039 | 1088540 | 20.0 |